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The layout of a 'Note' is the same as that of a paper. Short summaries are required.

The procedure for submission, administration, refereeing, editing and publication of 'Notes' is the same as for 'full' papers. However, 'Notes' are published more quickly than papers since their brevity facilitates processing at all stages.

The Editors endeavour to meet authors' wishes as to whether an article is a full paper or a 'Note', but since there is no sharp dividing line between the one and the other, either in terms of length or character of contents, the right is retained to transfer overlong 'Notes' to the 'full papers' section. As a guide a 'Note' should not exceed 1500 words or word-equivalents.

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For many years the Society has actively encouraged the use of standard IUPAC nomenclature and symbolism in its publications as an aid to the accurate and unambiguous communication of chemical information between authors and readers. In order to encourage authors to use IUPAC nomenclature rules when drafting papers, attention is drawn to the following publications in which both rules themselves and guidance on their use are given.

**Physicochemical Quantities and Units**

Manual of Symbols and Terminology for Physicochemical Quantities and Units. (*Pure and Appl. Chem.*, Vol. 51, No. 1, 1979, pp. 1–41. Also available as a soft-cover booklet from Pergamon Press, Oxford.)

**Surface Chemistry**

'Definitions, Terminology, and Symbols in Colloid and Surface Chemistry – I.' (*Pure and Appl. Chem.*, Vol. 31, No. 4, 1972, pp. 577–638.)

'Definitions, Terminology, and Symbols in Colloid and Surface Chemistry – II. Heterogeneous Catalysts.' (*Pure and Appl. Chem.*, Vol. 46, No. 1, 1976, pp. 71–90.)

—In addition, the terminology and symbols for the following subject areas are available either in the form of soft-cover booklets from Pergamon Press (denoted by *) or have been the subject of articles in *Pure and Applied Chemistry* in recent years: activities;* chromatography; electrochemistry; electron spectroscopy; equilibria, fluid flow; ion exchange; liquid–liquid distribution; molecular force constants; Mössbauer spectra; nuclear chemistry; pH; polymers; quantum chemistry; radiation;* Raman spectra; reference materials (recommended reference materials for the realisation of physicochemical properties: general introduction, enthalpy, optical rotation, surface tension, optical refraction, molecular weight, absorbance and wavelength, pressure–volume–temperature relationships, reflectance, potentiometric ion activities, testing distillation columns), solution chemistry; spectrochemical analysis; surface chemistry; thermodynamics, and zeolites.

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'Nomenclature of Organic Chemistry, Sections A, B, C, D, E, F, and H', 1979.

'Nomenclature of Inorganic Chemistry', 1971.

# Publication of Theoretical and Computational Papers

The Journals Committee has considered its policy towards the publication of papers with a heavily computational content, particularly where these involve standard methods, such as semi-empirical or *ab initio* calculations of molecular electronic properties using readily available computer programs. Many such papers report what would be considered 'routine work' in other areas of chemistry and have often included extensive detail.

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(i) Papers should be submitted to the appropriate journal: a paper containing innovations in theory to Faraday Transactions II, one in which the computations are incidental to the chemistry to Perkin, Dalton or Faraday I Transactions. Papers concerned mainly with computational details are unlikely to be accepted.

(ii) The purpose of the paper and the precise objectives of the calculations performed should be clearly stated: the results obtained should be reported only in so far as they relate to those objectives.

(iii) Many papers use a routine procedure based on a well documented method, be it semi-empirical or *ab initio*. It is then sufficient to name the particular variant, referring to key papers in which the method was developed, to cite the computer program used, and to indicate *briefly* any modification made by the author. A review of theoretical background would be out of place, but an author should say why he considers the method adequate for his purposes.

(iv) Extensive tabulation of numerical results, such as the magnitudes of atomic orbital coefficients, electron populations, contour maps of molecular orbitals and electron densities, and peripheral material of a similar nature, is normally unnecessary. Lengthy line-by-line discussion of such material is, as a general rule, quite unacceptable. Where an author considers that there is a special need to make such material available to other workers, as with highly accurate computations, for example, then this may be deposited with the British Library as a Supplementary Publication. Such material should be submitted with the main paper, clearly distinguished from it, and referred to in the main text.

Guidelines can never provide sufficient criteria for acceptance or rejection of a paper. Critical assessment of the theoretical methods used in a computation, and of their suitability for the purpose in hand, will continue to be entrusted to specialist referees who must also decide whether the results are new and advance science.

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The growing volume of research that produces large quantities of data, the increasing facilities for analysing such data mechanically, and the rising cost of printing are each making it very difficult to publish in the *Journal* in the normal way the full details of the experimental data which become available. Moreover, whilst there is a large audience for the general method and conclusions of a research project, the number of scientists interested in the details, and in particular in the data, of any particular case may be quite small. The British Library Lending Division (B.L.L.D.) in consultation with the Editors of scientific journals, has now developed a scheme whereby such data and detail may be stored and then copies made available on request at the B.L.L.D., Boston Spa. The Society is a sponsor of this scheme and has indicated to the B.L.L.D. its wish to use the facilities being made available in this 'Supplementary Publications Scheme'.

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